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Contact parameters in two dimensions for general three-body systems

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Abstract

We study the two-dimensional three-body problem in the general case of three distinguishable particles interacting through zero-range potentials. The Faddeev decomposition is used to write the momentum-space wave function. We show that the large-momentum asymptotic spectator function has the same functional form as derived previously for three identical particles. We derive the analytic relations between the three different Faddeev components for the three distinguishable particles. We investigate the one-body momentum distributions both analytically and numerically and analyze the tail of the distributions to obtain two- and three-body contact parameters. We specialize from the general cases to the examples of two identical, interacting or non-interacting, particles. We find that the two-body contact parameter is not a universal constant in the general case and show that the universality is recovered when a subsystem is composed of two identical non-interacting particles. We also show that the three-body contact parameter is negligible in the case of one non-interacting subsystem compared to the situation where all the subsystems are bound. As an example, we present the results for mixtures of lithium with two cesium or two potassium atoms, which are systems of current experimental interest.

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1. Introduction

The surprising and unexpected predictions from quantum mechanics have been challenging our classical intuition for a century. Since then, efforts in both the theoretical and experimental fields have increasingly aimed at a better understanding of quantum systems. In particular, experiments with cold atomic gases [1] are an interesting way of building and probing quantum systems: the properties of the atomic condensates near absolute zero temperature are governed by pure quantum effects. An interesting example of an unexpected quantum mechanical prediction that was experimentally confirmed in cold atomic gases is the so-called Efimov effect, which predicts that three identical bosons interacting through short-range potentials present infinitely many bound states, where the energies between the states are geometrically spaced. This effect was predicted by Efimov in 1970 [2] and was experimentally verified in cold atomic gases experiments in 2006 [3]. The Efimov effect happens for three-dimensional (3D) systems, while quantum theory predicts that the same two dimensional (2D) system presents only two bound states and no Efimov effect [4–8]. The theoretical difference arising from changing system dimension could most probably also be verified in cold atomic gases experiments in the near future since the experimentalists are already able to change the dimensionality of such systems and build experiments in effectively one (one dimensional (1D)) or two (2D) spatial dimensions.

Another important theoretical prediction, that was recently reported in [9], is the emergence of a parameter in the study of two-component Fermi gases, the two-body contact parameter, $C_2$, which connects the universal relations between the two-body correlations and the many-body properties [9–19]. This parameter can most easily be defined by considering the single-particle momentum distribution of the system, $n(q)$. In the limit where $q \to \infty$, one finds

$$\lim_{q \to \infty} q^4 n(q) = C_2.$$

(1)

As mentioned above, this parameter appears in a number of universal relations for both few- and many-body properties. These relations also hold for bosons and were confirmed in cold atomic gases experiments for the two-component Fermi gases [20, 21] and bosons [22]. One way to determine this parameter is to find the coefficient in the leading order asymptotic behavior of the one-body momentum density of the few-body systems. The next order in this expansion defines the three-body contact parameter, $C_3$, but since the Pauli principle suppresses the short-range correlations for the two-component Fermi gases, the three-body parameter is only important for the bosons [14, 18]. In a gas of identical bosons in 3D, the Efimov effect occurs and one finds a momentum distribution of the form

$$n(q) \to \frac{C_2}{q^4} + C_3 \frac{\sin(s_0 \ln(q) + \delta)}{q^5}$$

for $q \to \infty$,

(2)

where $s_0$ is the Efimov parameter [2] and $\delta$ is a constant [17].

The two- and three-body contact parameters were studied for a 3D system of three identical bosons in [16, 17, 23] and for the mixed-species systems in [24]. These results show that the influence of non-equal masses in the three-body systems goes beyond changing the contact parameter values. In 3D the sub-leading term, which defines $C_3$, changes to a different functional form when the masses are not equal. In view of that, one may ask what changes could we obtain
when dealing with the mixed-species systems in 2D. It is known that the mixed-species systems have a richer energy spectrum in 2D compared with the symmetric mass systems [25–27]. The study of the momentum distribution for three identical bosons in 2D was reported in [28], where the two-body contact parameter is found to be a universal constant, in the sense that $C^2_{E_3}$ is the same for both the three-body bound states of energy $E_3$. The leading order term of the momentum distribution at large momenta has the same inverse quartic form in 1D [29, 30], 2D and 3D. This can be derived on general grounds and is intuitively connected to the behavior of the free propagator for the particles [23, 31]. However, the three-body contact parameter and the functional form of the sub-leading term were shown to present very different behavior in 2D, compared with 3D [28], although no analytical results have been presented to estimate the value of the contact parameter.

In this paper, we study the cylindrically symmetric three-body bound states of the 2D systems composed for three distinguishable particles with attractive short-range interactions. We derive the analytic expressions for $C_2$ and $C_3$ and numerically obtain the one-body momentum density to verify our results. Unlike the 3D systems, the sub-leading order in the asymptotic momentum density presents the same functional form for both equal masses and mixed-species systems. We find that $C_2$ no longer shows universal behavior in the general case but that the universality is recovered in at least one special case of two identical non-interacting particles. We also extend our asymptotic formulae to the full range of the momenta and use it to give an analytic expression for $C_2$ for the ground state.

The paper is organized as follows. The formalism and the quantities that appear in the work are properly shown and defined in section 2. The analytic formulae for the asymptotic spectator function are discussed in section 3 and the one-body large momentum behavior is derived in section 4. The numerical results with an appropriate discussion are presented in section 5. Discussion, conclusions and an outlook are given in section 6.

2. Formalism

We consider the 2D problem of three interacting particles of masses $m_A$, $m_B$ and $m_C$, which are pairwise bound with energies $E_{AB}$, $E_{AC}$ and $E_{BC}$. The interaction is assumed to be described as attractive zero-range potentials and the resulting s-wave three-body bound state of energy $-E_3$ is fully determined by these six parameters: three two-body energies and the three masses. We shall only investigate the bound states and we therefore let $E_3 > 0$ denote the absolute value of the binding energy. We use the Faddeev decomposition to write the momentum space wave function as [32]

$$\Psi(\mathbf{q}_\alpha, \mathbf{p}_\alpha) = f_\alpha(q_\alpha) + f_\beta\left(p_\alpha - \frac{m_\beta}{m_\beta + m_\gamma}q_\alpha\right) + f_\gamma\left(p_\alpha + \frac{m_\gamma}{m_\beta + m_\gamma}q_\alpha\right) \frac{E_3 + \frac{q^2_\alpha}{2m_\beta + m_\gamma}}{E_3 + \frac{q^2_\alpha}{2m_\beta + m_\gamma} + \frac{p^2_\alpha}{2m_\gamma}},$$

(3)

where $\mathbf{q}_\alpha, \mathbf{p}_\alpha$ are the Jacobi momenta of the particle $\alpha$ and $m_{\beta\gamma,a} = m_\alpha(m_\beta + m_\gamma)/(m_\alpha + m_\beta + m_\gamma)$ and $m_{\beta\gamma} = (m_\beta + m_\gamma)/(m_\beta + m_\gamma)$ are the reduced masses. We use here $(\alpha, \beta, \gamma)$ as the cyclic permutations of $(A, B, C)$. The wave function is written in the Jacobi coordinate system related to the momentum, $\mathbf{q}_\alpha$, of the particle $\alpha$ relative to the center of mass of the $\beta$–$\gamma$ subsystem.
The three spectator functions, \( f_{\alpha, \beta, \gamma}(q) \), or the momentum space Faddeev components, obey the three coupled homogeneous integral equations for any given bound state \([32]\)

\[
f_{\alpha}(q) = \tau_{\alpha}(q, E3) \int d^{2}k \left( \frac{f_{\beta}(k)}{E3 + \frac{q^{2}}{2m_{\beta\gamma}} + \frac{k^{2}}{2m_{\beta\gamma}} + \frac{1}{m_{\gamma}}k \cdot q} + \frac{f_{\gamma}(k)}{E3 + \frac{q^{2}}{2m_{\beta\gamma}} + \frac{k^{2}}{2m_{\beta\gamma}} + \frac{1}{m_{\beta}}k \cdot q} \right),
\]

where

\[
\tau_{\alpha}(q, E3) = 4\pi m_{\beta\gamma} \ln \left( \frac{\sqrt{\frac{q^{2}}{2m_{\beta\gamma}u} + E3}}{E_{\beta\gamma}} \right)^{-1}.
\]

The equations of motion defining the spectator functions are seen to be invariant under the following scaling relations: (i) multiply all the energies, that is \(E3\) as well as all \(E_{\beta\gamma}\), by the same constant \(\tau_{c}\); and (ii) multiply all the masses by a constant factor \(s_{c}\). Then, all the momenta \((q_{\alpha}, p_{\alpha})\) should be multiplied by \(\sqrt{\tau_{c}s_{c}}\). This means that we can choose both a unit of energy, say \(E2\), and a unit of mass, say \(m_{2}\), while using the momenta in the unit of \(\sqrt{m_{2}E2}\). In other words, after all the calculations are done with \(E2 = 1\) and \(m_{2} = 1\), we have to multiply all the energies by \(E2\), all the masses by \(m_{2}\) and all the momenta by \(\sqrt{m_{2}E2}\). The one-body momentum density of particle \(\alpha\) is defined by \(n(q_{\alpha}) = \int d^{2}p_{\alpha}|\Psi(q_{\alpha}, p_{\alpha})|^{2}\), where \(\Psi(q_{\alpha}, p_{\alpha})\) is given in (3).

We use the normalization where \(\int d^{2}q_{\alpha} n(q_{\alpha}) = 1\). Following the procedure in \([17, 24, 28]\), we group the nine terms in \(\int d^{2}p_{\alpha}|\Psi(q_{\alpha}, p_{\alpha})|^{2}\) into four components with a distinctly different integrand structure. The one-body momentum density is expressed as a sum of four terms, that is \(n(q_{\alpha}) = \sum_{i=1}^{4} n_{i}(q_{\alpha})\).

A general system of three distinguishable particles presents the three distinct one-body momentum density distributions corresponding to the different particles. The four terms for the particle \(\alpha\) can be expressed as

\[
n_{1}(q_{\alpha}) = |f_{\alpha}(q_{\alpha})|^{2} \int d^{2}p \frac{1}{\left( E3 + \frac{q^{2}}{2m_{\beta\gamma}} + \frac{p^{2}}{2m_{\beta\gamma}} \right)^{2}} = 2\pi m_{\beta\gamma} \frac{|f_{\alpha}(q_{\alpha})|^{2}}{E3 + \frac{q_{\alpha}^{2}}{2m_{\beta\gamma}u}},
\]

\[
n_{2}(q_{\alpha}) = \int d^{2}k \frac{|f_{\beta}(k)|^{2}}{\left( E3 + \frac{q^{2}}{2m_{\beta\gamma}} + \frac{k^{2}}{2m_{\beta\gamma}} + \frac{1}{m_{\gamma}}k \cdot q \right)^{2}} + \int d^{2}k \frac{|f_{\gamma}(k)|^{2}}{\left( E3 + \frac{q^{2}}{2m_{\beta\gamma}} + \frac{k^{2}}{2m_{\beta\gamma}} - \frac{1}{m_{\beta}}k \cdot q \right)^{2}},
\]

\[
n_{3}(q_{\alpha}) = 2f_{\alpha}(q_{\alpha}) \left[ \int d^{2}k \frac{f_{\beta}(k)}{\left( E3 + \frac{q^{2}}{2m_{\beta\gamma}} + \frac{k^{2}}{2m_{\beta\gamma}} + \frac{1}{m_{\gamma}}k \cdot q \right)^{2}} + \int d^{2}k \frac{f_{\gamma}(k)}{\left( E3 + \frac{q^{2}}{2m_{\beta\gamma}} + \frac{k^{2}}{2m_{\beta\gamma}} - \frac{1}{m_{\beta}}k \cdot q \right)^{2}} \right],
\]

\[
n_{4}(q_{\alpha}) = \int d^{2}k \frac{f_{\beta}(k) f_{\gamma}(k) \left( k + q_{\alpha} \right)}{\left( E3 + \frac{q^{2}}{2m_{\beta\gamma}} + \frac{k^{2}}{2m_{\beta\gamma}} + \frac{1}{m_{\gamma}}k \cdot q \right)^{2}} + \int d^{2}k \frac{f_{\gamma}(k) f_{\beta}(k) \left( k + q_{\alpha} \right)}{\left( E3 + \frac{q^{2}}{2m_{\beta\gamma}} + \frac{k^{2}}{2m_{\beta\gamma}} - \frac{1}{m_{\beta}}k \cdot q \right)^{2}},
\]

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where the integration variables originating from (3) are properly redefined to simplify the arguments of the spectator functions in the integrands. Only $n_4$ is then left with an angular dependence through the spectator functions. We emphasize that the distributions for the other particles can be obtained by the cyclic permutations of $(\alpha, \beta, \gamma)$ in these expressions.

3. Spectator functions

The spectator functions are the key ingredients. They can be characterized by their behavior in the small and the large momentum limits. We are first of all interested in large momenta, but we shall also extract the behavior for small momenta. Hopefully, these pieces can be put together in a coherent structure.

3.1. Large-momentum behavior

For three identical bosons all the spectator functions are equal, and the large-momentum behavior was previously found to be \[ \lim_{q \to \infty} f(q) = \Gamma_0 \frac{\ln q}{q^2}, \] where the constant $\Gamma_0$ depends on which excited state we focus on. Corrections, $\delta f(q)$, to (10) must vanish faster than $\ln(q)/q^2$ for $q \to \infty$, i.e. $\delta f(q)/\ln(q) \to 0$. Henceforth, we will refer to (10) as the large-momentum leading order behavior of the spectator function.

For three distinct particles, we have three different spectator functions. However, their large-momentum asymptotic behavior remains identical, when all three two-body subsystems are bound, except for the individual proportionality factors. To prove this, we carry out the angular integrals in (4), which immediately gives

\[
\begin{align*}
    f_\alpha(q) &= 2\pi \tau_\alpha(q, E_3) \left[ \int_0^\infty dk \frac{k f_\beta(k)}{\left(E_3 + \frac{q^2}{2m_{\gamma\gamma}} + \frac{k^2}{2m_{\beta\gamma}}\right)} \sqrt{1 - \frac{k^2 q^2/m_\gamma^2}{\left(E_3 + \frac{q^2}{2m_{\alpha\gamma}} + \frac{k^2}{2m_{\beta\gamma}}\right)^2}} \\
    &+ \int_0^\infty dk \frac{k f_\gamma(k)}{\left(E_3 + \frac{q^2}{2m_{\alpha\beta}} + \frac{k^2}{2m_{\beta\gamma}}\right)} \sqrt{1 - \frac{k^2 q^2/m_\beta^2}{\left(E_3 + \frac{q^2}{2m_{\alpha\beta}} + \frac{k^2}{2m_{\beta\gamma}}\right)^2}} \right].
\end{align*}
\]  

The two terms in (11) have the same form, and one can be obtained from the other by interchange of $\beta$ and $\gamma$. It therefore suffices to calculate the first integral in (11).

The contribution for large $q$ can in principle be collected from the $k$-values ranging from zero to infinity. To separate the small and the large $k$-contributions we divide the integration into two intervals, that is from zero to a large ($q$-independent) momentum $\Lambda \gg \sqrt{E_3}$ and from $\Lambda$ to
infinity. Thus,

\[
f_a(q) = \tau_a(q, E_3) \left[ \int_0^\Lambda dk \frac{k f_\beta(k)}{\left(E_3 + \frac{q^2}{2m_\gamma} + \frac{k^2}{2m_\gamma}\right) \sqrt{1 - \frac{k^2 q^2/m_\gamma^2}{\left(E_3 + \frac{q^2}{2m_\gamma} + \frac{k^2}{2m_\gamma}\right)^2}} \right] \\
+ \int_\Lambda^\infty dk \frac{k f_\beta(k)}{\left(\frac{q^2}{2m_\gamma} + \frac{k^2}{2m_\gamma}\right) \sqrt{1 - \frac{k^2 q^2/m_\gamma^2}{\left(E_3 + \frac{q^2}{2m_\gamma} + \frac{k^2}{2m_\gamma}\right)^2}}} + \cdots ,
\]

where the dots indicate that the second term in (11) should be added. For \(q \to \infty\) the first term, \(f_{a,1}\), on the right-hand side of (12) goes to zero as

\[
\lim_{q \to \infty} f_{a,1}(q) \to \frac{m_\beta y}{2m_\gamma} \ln q \int_0^\Lambda \frac{dk}{\left(k \left(\frac{q^2}{2m_\gamma} + \frac{k^2}{2m_\gamma}\right) \sqrt{1 - \frac{k^2 q^2/m_\gamma^2}{\left(E_3 + \frac{q^2}{2m_\gamma} + \frac{k^2}{2m_\gamma}\right)^2}} \right)} ,
\]

where we used \(\tau_a(q, E_3) \to \left[2m_\gamma y \ln q\right]^{-1}\) and that both \(E_3\) and \(\frac{k^2}{2m_\gamma}\) are much smaller than \(\frac{q^2}{2m_\gamma}\). The integral in (13) is finite and only weakly \(q\)-dependent for large \(q \gg \Lambda\). The asymptotic spectator function in (10) can be inserted in the second term, \(f_{a,2}\), on the left-hand side of (12), because we are in the asymptotic limit where \(k > \Lambda\). For \(q \to \infty\) we then obtain

\[
\lim_{q \to \infty} f_{a,2}(q) \to \frac{\Gamma_\beta}{2m_\gamma y \ln q} \int_\Lambda^\infty \frac{dk}{k \left(\frac{q^2}{2m_\gamma} + \frac{k^2}{2m_\gamma}\right) \sqrt{1 - \frac{k^2 q^2/m_\gamma^2}{\left(E_3 + \frac{q^2}{2m_\gamma} + \frac{k^2}{2m_\gamma}\right)^2}}} \frac{\ln k}{q^2 \ln q} \int_{\Lambda/q}^\infty \frac{dy}{y} \frac{\ln y + \ln q}{y \left(m_\beta y + y^2\right)} ,
\]

where we changed the integration variable, \(k = q y\), in the last expression. Carrying out the two integrals we obtain

\[
\int_{\Lambda/q}^\infty \frac{dy}{y} \frac{\ln y}{y \left(m_\beta y + y^2\right)} = \frac{1}{2} \left[ \frac{\ln^2 y}{m_\beta y + y^2} \right]_{\Lambda/q}^\infty \\
+ \int_{\Lambda/q}^\infty \frac{dy}{y} \frac{y \ln^2 y}{m_\beta y + y^2} \frac{1}{2} \to -\frac{m_\beta y}{2m_\gamma} \ln^2 \left(\frac{\Lambda}{q}\right) \to -\frac{\ln^2 q}{2m_\gamma} ,
\]

\[
\int_{\Lambda/q}^\infty \frac{dy}{y} \frac{1}{y \left(m_\beta y + y^2\right)} = \left[ \frac{\ln y}{m_\beta y + y^2} \right]_{\Lambda/q}^\infty \\
+ 2 \int_{\Lambda/q}^\infty \frac{dy}{y} \frac{y \ln y}{m_\beta y + y^2} \to -m_\beta y \ln \left(\frac{\Lambda}{q}\right) \to \frac{\ln q}{m_\beta y} ,
\]
Figure 1. The difference \( f_\alpha(q) - \frac{\Gamma}{m_\beta} \ln q \) as a function of the momentum \( q \). We see that (19) exactly describes the asymptotic spectator function within our accuracy.

where we found that the integrals on the right-hand side of (16) and (17) are finite and their contributions can be neglected when \( q \to \infty \) in comparison with the terms maintained.

In total, the spectator functions in (11) are now found by inserting (16) and (17) in (15). Notice that the contribution from (17) has to be multiplied by \( \ln q \). With the \( \gamma - \beta \) interchange, we also get the second term on the right-hand side of (11). The leading order large-momentum behavior of the spectator functions is therefore

\[
\lim_{q \to \infty} f_\alpha(q) \to \left( \frac{m_\alpha}{2m_\beta} \Gamma_\beta + \frac{m_\alpha}{2m_\gamma} \Gamma_\gamma \right) \frac{\ln q}{q^2}. \tag{18}
\]

Replacing \( f_\alpha(q_\alpha) \) in (18) by its conjectured asymptotic form, (10), we find a system of three linear equations for the three unknowns, \( \Gamma_\alpha = \frac{m_\alpha}{2m_\beta} \Gamma_\beta + \frac{m_\alpha}{2m_\gamma} \Gamma_\gamma \), which can be rewritten as \( m_\beta \Gamma_\alpha = m_\alpha \Gamma_\beta = \Gamma_\gamma m_\alpha \beta := \Gamma \). The leading order large-momentum asymptotic behavior for the three spectator functions is then

\[
\lim_{q \to \infty} f_\alpha(q) \to \frac{\Gamma}{m_\beta} \ln q \frac{1}{q^2}. \tag{19}
\]

This result relates the asymptotic behavior of the three spectator functions for one state. The remaining constant \( \Gamma \) still depends on which excited state we consider, and furthermore, also on the two-body masses and the two-body energies.

The derived large-momentum asymptotic behavior and the coefficients in (19) beautifully agree with the numerical calculation. In figure 1, we plot the difference \( f_\alpha(q) - \frac{\Gamma}{m_\beta} \ln q \) as a
Figure 2. Ratios between the three distinct spectator functions for a generic case of three distinct particles. Discrete points are the ratios between the spectator functions numerically calculated through (4) and the full lines are the ratios between the coefficients in (19).

function of the momentum $q$ for the two different spectator functions for the $^{133}\text{Cs}^{133}\text{Cs}^{6}\text{Li}$ system. We also show the same difference for a different system with three identical bosons. Firstly, this demonstrates that the large-momentum behavior is always $\ln q/q^2$ for any 2D spectator function. Secondly, for a given state the three cyclic permutations of $f_\alpha(q)m_\beta\gamma$ for large $q$ approach the same constant $\Gamma$ times $\ln q/q^2$. This general large-momentum behavior is further demonstrated in figure 2 for a system of three distinct particles. The numerically calculated points are compared with the full lines obtained from (19). This comparison is again consistent with the derived asymptotic behavior, and furthermore exhibits the rate and the accuracy of the convergence. The limit is reached within 10 and 1% already for $q/\sqrt{m_AE_{AC}} \approx 50$ and $q/\sqrt{m_AE_{AC}} \approx 10^4$, respectively.

3.2. Parameterizing from small to large momenta

The asymptotic spectator function in (19) seems to be a good approximation even for moderate values of $q$, e.g. $q \approx 3\sqrt{E_3}$. We also have information about the large-distance behavior for a given binding energy, that is $\exp(-\kappa \rho)$, where $\kappa$ is related to the binding energy and $\rho$ is the hyperradius. Fourier transformation then relates to the small momentum limit with overall behavior of $(D + q^2)^{-1}$, where $D$ is a constant related to the energy. This perfectly matches (3)
when two Jacobi momenta are present as in the three-body system. We therefore attempt a parameterization by combining the expected small momenta with the known large-momentum behavior:

$$f_\alpha(q) = f_\alpha(0) \frac{E_3}{\ln(E_3)} \frac{\ln(\sqrt{\frac{q^2}{2m_{\beta\gamma,\alpha}} + E_3})}{\sqrt{\frac{q^2}{2m_{\beta\gamma,\alpha}} + E_3}},$$

(20)

where $f_\alpha(0)$ is a normalization constant that satisfies $\int d^2q_\alpha n(q_\alpha) = 1$.

We should first emphasize that excited states with the same angular structure must have different numbers of radial nodes. Therefore, we concentrate here only on the ground state. The expression in (20) for the three ground state spectator functions parameterizes the small momentum behavior almost perfectly for the case of three distinguishable particles. This is seen in figure 3 where we compare the numerical and the parameterized solutions. However, when the small momenta are reproduced, the large-momentum limit deviates in the overall normalization, although with the same $q$-dependence. Surprisingly, the analytic expression is most successful for the spectator function related to the heaviest particle in the three-body system. This large-momentum mismatch is due to the normalization choice in (20), which is chosen to exactly reproduce the $q = 0$ limit.
4. One-body large momentum density

The one-body density functions are observable quantities. The most directly measurable part is the limit of large momenta. We therefore separately consider the large-momentum limit of the four terms in (6)–(9). We employ the method sketched in [28] and used to present the numerical results for three identical bosons in 2D. Here, we shall give more details and generalize to the systems of three distinguishable particles.

In 3D, the corresponding problem was solved by inserting the asymptotic spectator function (19) into each of the four terms in (6)–(9), and by evaluating the corresponding integrals [17, 24]. This procedure is not guaranteed to work in 2D because momenta smaller than the asymptotic values may contribute in the integrands. However, for the 3D it was shown that the leading order in the integrands is sufficient to provide both the leading and the next-to-leading order of the one-body momentum distributions. The details of these calculations in 3D can be found in [17] for three identical bosons and in [24] for mass-imbalanced systems.

The large-momentum spectator functions change a lot as the dimensionality is changed, going from $\sin(\ln(q)/q^2)$ in 3D to $\ln(q)/q^2$ in 2D. If we try to naively proceed in 2D as we have successfully done in 3D, the integrals diverge. We can circumvent this divergence problem by following the procedure used in the derivation of the asymptotic spectator functions. In the following, we work out each of the four momentum components defined in (6)–(9). In addition, we must simultaneously consider the next-to-leading order term arising from the dominant $n_2$-term.

- $n_1(q_a)$. This term is straightforward to calculate. The argument of the spectator function in (6) does not depend on the integration variable. The large-momentum limit is then found by replacing the spectator function by its asymptotic form and taking the large $q$ limit after a simple integration. We then obtain

$$\lim_{q_a \to \infty} n_1(q_a) \to 4\pi m_{\beta\gamma,\alpha} m_{\beta\gamma} \frac{|f_{a}(q_a)|^2}{q_a^2} \to 4\pi m_{\beta\gamma,\alpha} m_{\beta\gamma} \Gamma_2 \ln^2(q_a) q_a^6. \quad (21)$$

- $n_2(q_a)$. We integrate the two terms in (7) over the angle as allowed by the simple structure where the spectator function is angle independent. The result

$$n_2(q_a) = 2\pi \int_{0}^{\infty} dk \frac{k \left| f_{\beta}(k) \right|^2 \left( E_3 + \frac{k^2}{2m_{\gamma\beta}} + \frac{k^2 q_a^2}{2m_{\nu\gamma}} \right)}{\left[ \left( E_3 + \frac{k^2}{2m_{\gamma\beta}} + \frac{k^2 q_a^2}{2m_{\nu\gamma}} \right)^2 - \frac{k^2 q_a^2}{m_{\nu\gamma}} \right]^{3/2}}$$

$$+ 2\pi \int_{0}^{\infty} dk \frac{k \left| f_{\gamma}(k) \right|^2 \left( E_3 + \frac{k^2}{2m_{\nu\gamma}} + \frac{k^2 q_a^2}{2m_{\gamma\beta}} \right)}{\left[ \left( E_3 + \frac{k^2}{2m_{\nu\gamma}} + \frac{k^2 q_a^2}{2m_{\gamma\beta}} \right)^2 - \frac{k^2 q_a^2}{m_{\nu\gamma}} \right]^{3/2}}. \quad (22)$$
is then expanded for large $q$. Since $\int_0^\infty dk \ k |f_a(k)|^2$ is finite, the large-momentum expansion becomes

$$\lim_{q_a \to \infty} n_2(q_a) \to \frac{8\pi}{q_a^3} \left( m_{a\gamma}^2 \int_0^\infty dk \ k |f_\beta(k)|^2 + m_{a\beta}^2 \int_0^\infty dk \ k |f_\gamma(k)|^2 \right) + n_5(q_a) \equiv \frac{C_{\beta\gamma}}{q_a^4} + n_5(q_a),$$

(23)

where the last equality defines $C_{\beta\gamma}$, which we call the two-body contact parameter for the $\beta\gamma$ two-body system. The second term on the right-hand side, $n_5(q_a)$, gives the next-to-leading term in the expansion of $n_3(q_a)$. It turns out that this term has the same asymptotic behavior as $n_3(q_a)$ and $n_4(q_a)$. We must consequently keep it, but we postpone the derivation. We emphasize that the one-body large-momentum leading order comes only because the main contribution to $\int_0^\infty dk \ k |f_a(k)|^2$ arises from the small $k$. This replacement would therefore lead to a completely wrong result. However, this is not always the case, as we shall see later for $n_5(q_a)$.

• $n_3(q_a)$. The structure of the $n_3(q_a)$ in (8) is similar to the $n_2(q_a)$ in (7). The only difference is that the spectator function under the integration sign now is not squared. This small functional difference leads to a completely different result. As in the previous case, we can still carry out the angular integration, which only involves the denominator. Integrating (8) over the angle we obtain

$$n_3(q_a) = 4\pi f_a(q_a) \int_0^\infty dk \ k f_\beta(k) \left( E_3 + \frac{q_\gamma^2}{2m_{a\gamma}} + \frac{k^2}{2m_{\beta\gamma}} \right) \left[ \left( E_3 + \frac{q_\gamma^2}{2m_{a\gamma}} + \frac{k^2}{2m_{\beta\gamma}} \right)^2 - \frac{k^2 q_\gamma^2}{m_{\gamma}^2} \right]^{3/2}$$

$$+ \int_0^\infty dk \ k f_\gamma(k) \left( E_3 + \frac{q_\beta^2}{2m_{a\beta}} + \frac{k^2}{2m_{\beta\gamma}} \right) \left[ \left( E_3 + \frac{q_\beta^2}{2m_{a\beta}} + \frac{k^2}{2m_{\beta\gamma}} \right)^2 - \frac{k^2 q_\beta^2}{m_{\beta}^2} \right]^{3/2}.$$  

(24)

Here, the difference between $n_2$ and $n_3$ becomes important, since $\int_0^\infty dk \ k f(k)$ is divergent and we cannot expand (24) as we did for (22). We shall instead proceed as we did in obtaining the asymptotic spectator function. We divide the integration in (24) at a large, but finite, momentum, $\Lambda \gg \sqrt{E_3}$, and each term on the right-hand side is split into two others. The two terms only differ by simple factors, and we therefore only give details for the first term. Changing variables to $k = q_a y$, (24) becomes

$$\lim_{q_a \to \infty} n_3(q_a) \to 16\pi m_{\beta\gamma}^2 f_a(q_a) \int_0^{\Lambda/q_a} dy \ y f_\beta(q_a y) \left( \frac{2m_{\beta\gamma} E_3}{q_a^2} + \frac{m_{\beta\gamma}}{m_{a\gamma}} + y^2 \right) \left[ \left( \frac{2m_{\beta\gamma} E_3}{q_a^2} + \frac{m_{\beta\gamma}}{m_{a\gamma}} + y^2 \right)^2 - \frac{4m_{\beta\gamma}^2}{m_{a\gamma}^2} y^2 \right]^{3/2}$$

$$+ 16\pi m_{\beta\gamma}^2 f_a(q_a) \Gamma \int_{\Lambda/q_a}^{\infty} dy \ y f_\gamma(q_a y) \left( \frac{m_{\beta\gamma}}{m_{a\gamma}} + y^2 \right) \left[ \left( \frac{m_{\beta\gamma}}{m_{a\gamma}} + y^2 \right)^2 - \frac{4m_{\beta\gamma}^2}{m_{a\gamma}^2} y^2 \right]^{3/2} + \cdots.$$  

(25)
where \( f_\beta(k) \) is replaced by its asymptotic form and \( E_3 \) is neglected in the second term on the right-hand side, where \( \sqrt{E_3} \ll \Lambda \) and \( k > \Lambda \). In the limit \( q_\alpha \to \infty \), the integral vanishes in the first term, which therefore does not contribute to the large-momentum limit. The integrals in the second term are

\[
\int_{\Lambda/q_\alpha}^\infty \frac{dy}{y} \ln \left( \frac{h(y)}{y} \right) = \frac{1}{2} \ln^2 \left( \frac{h(y)}{y} \right) \bigg|_{\Lambda/q_\alpha}^\infty - \frac{1}{2} \int_{\Lambda/q_\alpha}^\infty \frac{dy}{y} \ln^2(y) g(y)
\]

\[
\to - \frac{m^2_{\alpha\gamma}}{2m^2_{\beta\gamma}} \ln^2 \left( \frac{\Lambda}{q_\alpha} \right) \to - \frac{\ln^2(q_\alpha)}{2m^2_{\alpha\gamma}}, \quad (26)
\]

\[
\int_{\Lambda/q_\alpha}^\infty \frac{dy}{y} h(y) = \ln(y) h(y) \bigg|_{\Lambda/q_\alpha}^\infty - \int_{\Lambda/q_\alpha}^\infty \frac{dy}{y} \ln(y) g(y) \to - \frac{m^2_{\alpha\gamma}}{m^2_{\beta\gamma}} \ln \left( \frac{\Lambda}{q_\alpha} \right) \to \frac{\ln(q_\alpha)}{m^2_{\alpha\gamma}}, \quad (27)
\]

where

\[
h(y) = \left( \frac{m_{\beta\gamma}}{m_{\alpha\gamma}} + y^2 \right) \left[ \left( \frac{m_{\beta\gamma}}{m_{\alpha\gamma}} + y^2 \right)^2 - \frac{4m^2_{\beta\gamma}}{m^2_\gamma} y^2 \right]^{-3/2}, \quad (28)
\]

\[
g(y) = \frac{dh(y)}{dy}, \quad \lim_{y \to 0} \ln^2(y) g(y) \to 0, \quad \lim_{y \to \infty} \ln^2(y) g(y) \to 0. \quad (29)
\]

The function \( g(y) \) and its limits ensure that the integrals on the right-hand side of equations (26) and (27) are finite and their contributions to the momentum distribution can be neglected when \( q_\alpha \to \infty \). Finally, by inserting the results given in (26) and (27) into (25) and replacing the spectator function \( f_\alpha(q_\alpha) \) by its asymptotic form, the leading order term of the one-body momentum distribution from \( n_3(q_\alpha) \) is given by

\[
\lim_{q_\alpha \to \infty} n_3(q_\alpha) \to 8\pi \left( \frac{m_{\alpha\gamma} + m_{\alpha\beta}}{m_{\beta\gamma}} \right) \Gamma^2 \ln^3(q_\alpha) \frac{q^6_\alpha}{q^6_\alpha}, \quad (30)
\]

where the second term on the right-hand side of (24) is recovered and added by the interchange of \( m_{\alpha\gamma} \to m_{\alpha\beta} \) in (25)–(27).

Although \( n_2(q_\alpha) \) and \( n_3(q_\alpha) \) have rather similar forms, their contributions to the one-body large momentum density are quite different. As we shall see later, the next-to-leading order, \( n_5(q_\alpha) \), of \( n_2(q_\alpha) \) is comparable with the \( n_3(q_\alpha) \) leading order, given in (30).

- \( n_4(q_\alpha) \). This is the most complicated of the four additive terms in the one-body momentum density. The angular dependence in both the spectator arguments cannot be removed simultaneously by variable change. The formulation in (9) has the advantage that the argument in \( f_\gamma ((k + q_\alpha)) \) (or in \( f_\beta ((k + q_\alpha)) \)) is never small in the limit of large \( q_\alpha \). This is in contrast to a choice of variables where the numerator in the first term of (9) would be \( f_\gamma (k) f_\beta ((k - q_\alpha)) \), and the argument in \( f_\beta \) would consequently be small as soon as \( k \) is comparable with \( q_\alpha \). The main contribution to the integrals in (9) arises from the small \( k \).
For large $q_\alpha$, we can then use the approximation, $f_\gamma(|\mathbf{k} + \mathbf{q}_\alpha|) \approx f_\gamma(q_\alpha)$ (or $f_\beta(|\mathbf{k} + \mathbf{q}_\alpha|) \approx f_\beta(q_\alpha)$). The integrals are then identical to the terms of $n_3$ in (8). By keeping track of the slightly different mass factors we therefore immediately obtain the asymptotic limit to be

$$\lim_{q_\alpha \to \infty} n_4(q_\alpha) \to 4\pi \left( \frac{m_{a\gamma}}{m_{a\beta}} + \frac{m_{a\beta}}{m_{a\gamma}} \right) \Gamma^2 \ln^3(q_\alpha)/q_\alpha^6. \quad (31)$$

- $n_5(q_\alpha)$. This is the next-to-leading order contribution from the $n_2(q_\alpha)$ term. It turns out that this term has the same large-momentum behavior as the leading orders of both $n_3(q_\alpha)$ and $n_4(q_\alpha)$. By definition we have

$$n_5(q_\alpha) = n_2(q_\alpha) - \lim_{q_\alpha \to \infty} n_2(q_\alpha) = n_2(q_\alpha) - \frac{C_{\beta\gamma}}{q_\alpha^4}, \quad (32)$$

which can be rewritten in detail as

$$n_5(q_\alpha) = \lim_{q_\alpha \to \infty} 2\pi \int_0^\infty dk k \left| f_\beta(k) \right|^2 \left( \frac{E_3 + \frac{q_\alpha^2}{2m_{a\gamma}} + \frac{k^2}{2m_{a\gamma}}}{\left[ E_3 + \frac{q_\alpha^2}{2m_{a\gamma}} + \frac{k^2}{2m_{a\gamma}} \right]^2 - \frac{k^2 q_\alpha^2}{m_{a\gamma}^2}} \right)^{3/2} - \frac{4m_{a\gamma}^2}{q_\alpha^4} + \cdots, \quad (33)$$

where the dots denote the last term in (22) obtained by the interchange of $\beta$ and $\gamma$. The tempting procedure is now to expand the integrand around $q_\alpha = \infty$ assuming that $q_\alpha$ overwhelms all the terms in this expression. This immediately leads to the integrals corresponding to the cubic moment of the spectator function, which, however, is not converging. On the other hand, (33) is perfectly well defined due to the large-$k$ cut-off from the denominator. In fact, the spectator function is multiplied by $k^3$ and $1/k^3$ at the small and large $k$-values, respectively. The integrand therefore has a maximum where the main contribution to $n_5$ arises. This peak in $k$ moves toward the infinity proportional to $q$. To compute $n_5(q_\alpha)$ we then divide the integration into two intervals, that is from zero to a finite but very large $k$-value, $\Lambda_s$, and from $\Lambda_s$ to infinity. The small momentum interval, $k/q_\alpha \ll 1$, allows an expansion in $k/q_\alpha$ leading to the following contribution $n_{5,1}(q_\alpha)$:

$$n_{5,1}(q_\alpha) = 8\pi \frac{m_{a\gamma}^2}{q_\alpha^6} \left( \frac{3m_{a\gamma}^2}{m_{a\gamma}^2} - \frac{m_{a\gamma}}{m_{a\gamma}^2} \right) \int_0^{\Lambda_s} dk k^3 \left| f_\beta(k) \right|^2 + \frac{\eta}{q_\alpha^8} + \cdots, \quad (34)$$

where $\eta$ is a constant. Thus, the contribution from this small momentum integration vanishes with the sixth power of $q_\alpha$, which is faster than the other sub-leading orders we want to keep. We choose $\Lambda_s$ sufficiently large for the spectator function to reach its asymptotic behavior in (19). The large interval integration can now be performed by omitting the small $E_3$-terms and the change of the integration variable to $y$, $k^2 = yq_\alpha^2$, i.e.

$$n_{5,2}(q_\alpha) = \frac{\pi \Gamma^2}{q_\alpha^6} \int_0^{\infty} \frac{dy}{y^2} \left[ \ln^2(y) + 2 \ln y \ln(q_\alpha^2) \right] \times \left( \frac{1 + y m_{a\gamma}/m_{a\gamma}}{\left[ (1 + y m_{a\gamma}/m_{a\gamma})^2 - 4 y m_{a\gamma}^2 / m_{a\gamma}^2 \right]^{3/2}} - 1 \right) + \cdots, \quad (35)$$

where the large $y$-limit behaves like $\ln^2(y)/y^4$ and therefore ensures rapid convergence, whereas the integrand for small $y$ behaves like $(\ln^2(y) + \ln^2(q_\alpha^2) + 2 \ln y \ln(q_\alpha^2))/y$. Thus,
the integration from an arbitrary minimum value, \( y_L \) (independent of \( q_\alpha \)), of \( y > \Lambda^2/q_\alpha^2 \) yields a \( q_\alpha \)-independent value except for the logarithmic factors and \( q_\alpha \) in the numerator. Thus, the large-\( q_\alpha \) dependence is found from the very small values of \( y \) close to the lower, and vanishing, limit. In total, we obtain by expansion in small \( y \) that the limit for large \( q_\alpha \) approaches zero as

\[
\lim_{q_\alpha \to \infty} n_{5,2}(q_\alpha) \to \frac{16\pi \Gamma^2}{q_\alpha^6} \left( \frac{m_{\alpha\gamma}^2}{m_\gamma^2} - \frac{m_{\alpha\beta}}{m_\beta^2} \right) \int_{\Lambda^2/q_\alpha^2}^{y_L} dy \left[ \ln^2(y) + \ln^2(q_\alpha^2) + 2 \ln y \ln(q_\alpha^2) \right].
\]

(36)

Together with the term from the interchange of \( \beta \) and \( \gamma \) in (19) we obtain in total that

\[
\lim_{q_\alpha \to \infty} n_5(q_\alpha) \to \frac{16\pi}{3} \left[ \frac{m_{\alpha\gamma}^2}{m_\gamma^2} + \frac{m_{\alpha\beta}^2}{m_\beta^2} - \frac{m_{\alpha\gamma} m_{\alpha\beta}}{m_\gamma m_\beta} \right] \Gamma^2 \frac{\ln^3(q_\alpha)}{q_\alpha^6}.
\]

(37)

5. Two- and three-body contact parameters

We first collect the analytically derived relations, and secondly we compare them with numerically calculated values.

5.1. Analytic expressions

Two- and three-body contact parameters are defined via the large-momentum one-body density. The two-body contact parameter, \( C_{\beta\gamma} \), is the proportionality constant of the leading order \( q^{-4} \) term, which arises solely from \( n_2(q_\alpha) \) in (23). For three distinguishable particles we have three contact parameters each related to the momentum distribution of one particle. The definition is already given in (23). They are related through

\[
C_{\alpha\beta} + C_{\alpha\gamma} = C_{\beta\gamma} + \frac{16\pi}{3} \left[ \frac{m_{\alpha\gamma}^2}{m_\gamma^2} + \frac{m_{\alpha\beta}^2}{m_\beta^2} - \frac{m_{\alpha\gamma} m_{\alpha\beta}}{m_\gamma m_\beta} \right] \Gamma^2 \frac{\ln^3(q_\alpha)}{q_\alpha^6}.
\]

(38)

and the cyclic permutations. For a specific system, where two of the particles are non-interacting in 2D, the corresponding two-body energy vanishes, \( E_{\beta\gamma} = 0 \) [32, 33]. Then, from (4) the spectator function also vanishes, \( f_\alpha(q) = 0 \), and (38) reduces to

\[
C_{\alpha\beta} + C_{\alpha\gamma} = C_{\beta\gamma} \quad \text{for} \quad E_{\beta\gamma} = 0.
\]

(39)

In this case, we have this simple relation between the three two-body contact parameters. This relation between the different two-body parameters does not depend on the system dimension. Although our calculations are in 2D, this relation in (39) applies as well for 3D systems with one non-interacting subsystem. We emphasize that a non-interacting system and a vanishing two-body energy are not the same in 3D, where some attraction is necessary to provide a state with zero binding energy.

The three-body contact parameter, \( C_{\beta\gamma,\alpha} \), is defined as the proportionality constant on the next-to-leading order in the one-body large-momentum density distribution. For distinguishable particles we have again three of these parameters, each related to one of the particle’s momentum distributions. The asymptotic behavior, \( \ln^3(q_\alpha)/q_\alpha^6 \), receives contributions from the three terms specified in (30), (31) and (37). In total, we have

\[
C_{\beta\gamma,\alpha} = 16\pi \left( \frac{m_{\alpha\gamma} + m_{\alpha\beta}}{6m_{\beta\gamma}} + \frac{m_{\alpha\gamma}}{4m_{\alpha\beta}} + \frac{m_{\alpha\beta}}{4m_{\alpha\gamma}} + \frac{m_{\alpha\gamma}^2}{m_\gamma^2} + \frac{m_{\alpha\beta}^2}{m_\beta^2} \right) \Gamma^2.
\]

(40)
It is worth emphasizing that only a logarithmic factor distinguishes the behavior of the three-body contact term from the next order, $\ln^2(q_\alpha)/q_\alpha^6$, which arises from $n_1$ as well as from $n_2$, $n_3$ and $n_5$. In practical measurements, it must be a huge challenge to distinguish between terms differing by only one power of $\ln(q_\alpha)$.

For the three-body contact parameter, (40), with only one non-interacting two-body system, we obtain

$$C_{\beta\gamma,a} = 16\pi \left( \frac{m_{\alpha\gamma} + m_{a\beta}}{3m_{\beta\gamma}} + \frac{m_{\alpha\gamma} + m_{a\beta}}{4m_{\alpha\gamma}} + \frac{m_{\alpha\gamma} + m_{a\beta}}{m_{\gamma}} + \frac{m_{\alpha\gamma} + m_{a\beta}}{m_{\beta}} \right) \Gamma^2,$$

which is obtained by collecting the contributions from only the non-vanishing $n_4$ and $n_5$ terms (since $f_a(q) = 0$, $n_1$ and $n_3$ do not contribute). Cyclic permutations of the indices in (40) and (41) now allow the conclusion that the three different three-body contact parameters are related by the mass factors in (40) and (41). This conclusion holds for all the excited states. Universality of independence of the excited state is another matter and in fact not found numerically.

5.2. Numerical results

The results in the preceding subsection hold for any mass-imbalanced three-body system. Such a system has six independent parameters, which are reduced to four by choosing one mass and one energy as the units [33]. This merely implies that all the results can be expressed as ratios of masses and energies, in this way providing very useful scaling relations. Results depending on the four independent parameters are still hard to display and digest.

To build up our understanding, we now focus on systems composed of two identical particles, A, and a distinct one, C. Such a system has four independent parameters from the beginning, which are reduced to two after the choice of the units. From now on, we shall use $E_{AC}$ and $m_A$ as our energy and mass units, and for simplicity we introduce the mass ratio $m = m_C/m_A$.

In these units, the energies and the momenta appearing in the equations must be multiplied by $E_{AC}$ and $\sqrt{m_A E_{AC}}$, respectively. For this system the two-body contact parameters in (38) are given by

$$C_{AA} = 16\pi \left( \frac{m}{1+m} \right)^2 \int_0^\infty dk \, k |f_A(k)|^2,$$

$$C_{AC} = \frac{C_{AA}}{2} + 2\pi \int_0^\infty dk \, k |f_C(k)|^2.$$

For three identical particles where all the masses and the interactions are the same, $C_{AA} = C_{AC} = C_2$, and the quantity $C_2/E_1$ is a universal constant in 2D [18, 28]. To be explicit, this quantity has the same value for the only two existing bound states, ground and the first excited state. Mass-imbalanced systems have a richer energy spectrum with many excited states [27, 33]. Maintaining the universal conditions for all the excited states is obviously more demanding.

Detailed investigations reveal that when the mass–energy symmetry is broken, the universality of $C_2/E_1$ does not hold any more. The two two-body contact parameters defined in (42) and (43) divided by the three-body energy are not the same for all the possible bound states in the general case. However, in at least one special case of the two identical non-interacting particles, $E_{AA} = 0$, the universality is recovered. This is implied by $f_C = 0$ as seen from the
Figure 4. The leading order of the one-body momentum density divided by $E^n$ for each bound state labeled as $n$ in a system composed of two identical ($A = ^{133}\text{Cs}$) particles and a distinct one ($C = ^{6}\text{Li}$) as a function of the momentum $q$ for both $E_{AA} = 1$ and 0.

set of coupled homogeneous integrals equations (4). Then the two universal two-body contact parameters are related, that is

$$C_{AC} = \frac{C_{AA}}{2} \quad \text{for} \quad E_{AA} = 0.$$  \hspace{1cm} (44)

We illustrate in figure 4 how the two-body contact parameters vary with the excitation energy for a mass-asymmetric system. We choose $^{133}\text{Cs} - ^{133}\text{Cs} - ^{6}\text{Li}$ corresponding to $A = ^{133}\text{Cs}$ and $C = ^{6}\text{Li}$. This system has four excited states at the energies depending on the size of $E_{AA}$, and the large-momentum limit of the constants is reached in all cases. For $E_{AA} = 0$, the universality is observed, since all the two-body contact values, $C_{AC}/E_3$, are equal in the units of the three-body energy. This case is rather special because the two particles do not interact and the three-body structure is determined by the identical two-body interactions between the other two subsystems. In other words, the large-momentum limit of particle $A$ is determined universally by the properties of the $A$–$C$ subsystem. The other contact parameter, $C_{AA}/E_3$, is also universal and follows from (44).

This picture changes when all the particles interact, as seen in figure 4 for $E_{AA} = 1$. Now, the large-momentum limit, the constants still independent of the momentum, changes with the excitation energy. The systematics is that both $C_{AA}/E_3$ and $C_{AC}/E_3$ as the functions of the excitation energy move toward the corresponding values for $E_{AA} = 0$, one from below and the other from above. First, the non-universality is understandable, since the interaction of the two identical particles now must affect the three-body structure at small distances, and hence at large momenta. However, as the three-body binding energy decreases, the size of the system increases and the details of the short-distance structure become less important.
The quantities $\frac{C_{\text{AC}}}{E_3}$ and $\frac{2\pi}{E_3} \int_0^\infty dk \ |f_C(k)|^2$ are defined by the limiting large-$q$ behavior of $n_2$ in (23). Plotting the corresponding pieces of $n_2(q)q^4$ as a function of $q$ leads to figures very similar to figure 4, where different excitation dependent lines emerge for $E_{\text{AA}} = 1$, while they all coincide for $E_{\text{AA}} = 0$. The constant values for $\frac{C_{\text{AC}}}{E_3}$, $\frac{C_{\text{AA}}}{E_3}$ and $\frac{2\pi}{E_3} \int_0^\infty dk \ |f_C(k)|^2$ in the limit $q \to \infty$ are shown in table 1 for two different interactions and two different systems represented by $C = ^6\text{Li}$ and $A = ^{133}\text{Cs}$ or $A = ^{39}\text{K}$. These results of the numerical calculations confirm the systematics described above in complete agreement with (43) and (44).

In general, for two identical particles the two-body contact parameters divided by the three-body energy depend on the mass ratio $m$. The dependence changes from universal for $E_{\text{AA}} = 0$ to non-universal for $E_{\text{AA}} = 1$. The mass dependence for the ground states is shown in figure 5, where we see that the ratio $\frac{C_{\text{AA}}}{C_{\text{AC}}} = 2$ in (44) holds for $E_{\text{AA}} = 0$ in the entire mass interval investigated. We also see how the second term on the right-hand side of (43) affects the relation between the two two-body contact parameters. Figure 5 shows that the values rapidly increase from small $m$ up to 1 and become almost constant above $m \approx 5$. This behavior is similar to the mass-imbalanced system in the 3D [24].

We can estimate the two-body contact parameter dependence on the excitation energy by use of the approximation to the ground state in (20). In (42) we find inserted an expression for $\frac{C_{\text{AA}}}{E_3}$, that is

$$\frac{C_{\text{AA}}}{E_3} = 16\pi \frac{m^2}{(1+m)(2+m)} f_A^2(0) \left( \frac{2}{\ln(E_3)} + \frac{2}{\ln^2(E_3)} \right).$$

A comparison between this approximation and the numerical results is shown in figure 6. We see that (45) provides a fairly good estimate, which is accurate within 5% for small $m$, around 10% for $m > 1$ and within about 20% deviation in the worst case of $m = 1$. The divergence in (45) for $E_3 \to 1$ means that the two-body contact parameters diverge when the three-body system approaches this threshold of binding. This does not reveal the full energy dependence since the normalization factor, $f_A^2(0)$, also is state and energy dependent.

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**Table 1.** The constant values for the scaled two-body contact parameters $\frac{C_{\text{AC}}}{E_3}$, $\frac{C_{\text{AA}}}{E_3}$ and $\frac{2\pi}{E_3} \int_0^\infty dk \ |f_C(k)|^2$ in the limit $q \to \infty$ are shown for the two different interactions and the two different systems represented by $C = ^6\text{Li}$ and $A = ^{133}\text{Cs}$ or $A = ^{39}\text{K}$. The values in the fifth column are plotted in figure 4.

| System | $\frac{E_{\text{AA}}}{E_3}$ | State | $\frac{C_{\text{AA}}}{E_3}$ | $\frac{C_{\text{AC}}}{E_3}$ | $\frac{2\pi}{E_3} \int_0^\infty dk \ |f_C(k)|^2$ |
|--------|----------------|-------|----------------|----------------|----------------------------------|
| $A = ^{133}\text{Cs}$ $C = ^6\text{Li}$ | 1 | Ground | 0.02210 | 0.07625 | 0.06503 |
|        |        | First  | 0.02495 | 0.04062 | 0.02812 |
|        |        | Second | 0.02616 | 0.02612 | 0.01305 |
|        |        | Third  | 0.02718 | 0.01837 | 0.00478 |
|        | 0 | All    | 0.02748 | 0.01374 | 0.0 |
| $A = ^{39}\text{K}$ $C = ^6\text{Li}$ | 1 | Ground | 0.06337 | 0.11499 | 0.08372 |
|        |        | First  | 0.07438 | 0.08256 | 0.04727 |
|        |        | Second | 0.07934 | 0.05369 | 0.01840 |
|        | 0 | All    | 0.08304 | 0.04152 | 0.0 |

---
Figure 5. The two-body parameters $C_{AA}$ and $C_{AC}$ defined in (23) as a function of the mass ratio $m = \frac{m_C}{m_A}$ for an AAC system in both cases where $E_{AA} = 0$ and $E_{AC}$.

The non-universality of the two-body contact parameters does not encourage universality investigations of the three-body contact parameter, which is related to a sub-leading order. However, at least the system with two non-interacting identical particles turned out to be universal and may lead to an interesting large-momentum three-body structure. As before, by inserting $E_{AA} = 0$ in the set of coupled integral equations (4) we find $f_C(q_C) = 0$. Then, (6)–(9) show directly that $n_1(q_c)$ and $n_3(q_C)$ vanish when $f_C(q_C) = 0$, leaving only possible contributions from $n_4(q_C)$ and $n_5(q_C)$.

We show in figure 7 the sub-leading order of the large-momentum distribution multiplied by $q_C^6/\ln^3(q_C)$, that is $C_{AA,C}$, as functions of $q_C$ for the four bound states for a system where $A = ^{133}\text{Cs}$ and $C = ^6\text{Li}$ and for both $E_{AA} = 1$ and $E_{AA} = 0$. We only show one of these three-body contact parameters defined in (40) and (41) since the other one, $C_{AC,A}$, is related state-by-state through the mass factors in (40) and (41). The momentum dependence approaches the predicted constancy at large $q_C$ by increasing or decreasing for the interacting or the non-interacting identical particles, respectively. We divided by the three-body energy to see if a simple energy scaling could explain the differences. Not surprisingly, more complicated and non-universal behavior is present.

However, it is striking to see that this sub-leading order in the large-momentum limit is negligibly small for the non-interacting compared with the interacting identical particles. This implies that a negligible three-body contact parameter combined with a universal two-body
contact parameter can be taken as a signature of a two-body non-interacting subsystem within a three-body system in 2D.

6. Discussion and outlook

In this work, we have considered three-body systems with attractive zero range interactions for general masses and interaction strengths in 2D using the Faddeev decomposition to write the momentum-space wave function, through which the one-body momentum density is obtained. The momentum density tail gives the two- and the three-body contact parameters, namely $C_2$ and $C_3$, respectively. We derived the analytic expressions for the asymptotic spectator functions and for both $C_2$ and $C_3$ for three distinguishable bosons.

We found that the asymptotic spectator function for each of the three distinguishable particles has the same functional form as calculated for the three identical particles in [28]. Moreover, we showed that the three distinct spectator functions relate to each other through a constant, $\Gamma$, properly weighted by the reduced masses. These analytic results are supported by an accurate numerical calculation, which confirmed both the asymptotic behavior and the relation between the asymptotic expressions for different spectator functions in a generic case of the three distinguishable particles.
Figure 7. The sub-leading order of the one-body momentum density divided by $E_n^3$ for each bound state labeled as $n$ in a system composed of two identical (A = $^{133}$Cs) particles and a distinct one (C = $^6$Li) as a function of the momentum $q$ for both $E_{AA} = 1$ and 0.

The spectator functions and their asymptotic behavior define both the two- and the three-body contact parameters, $C_2$ and $C_3$. The parameter $C_2$ arises from integration of the spectator functions over all momenta, and both the small and the large momenta contribute. In the case of the ground state, we are able to use our knowledge of the asymptotics of the spectator function to infer the behavior for all the momenta. We found that the three two-body parameters for a system of three distinguishable particles are related by simple mass scaling. However, these two-body contact parameters are in general not universal in the sense of being independent of the state when more than one excited state is present. In contrast, we find universality for the three-body systems with one distinguishable and two identical, non-interacting particles. In that case the third particle apparently does not disturb the short-distance structure arising from the two interacting particles. Hence, the two-body contact parameter turn out to be universal. This is similar to the 3D case and the three identical bosons where $C_2$ is universal in the scaling or Efimov limit where the binding energy is negligible [17].

In 3D systems, the two-body contact has been observed in experiments using time-of-flight and the mapping to momentum space [20], Bragg spectroscopy [20–22, 34, 35] or momentum-resolved photoemission spectroscopy (similar to angle-resolved photoemission spectroscopy) [36]. Measuring the sub-leading term and thus accessing $C_3$ requires more precision, which has so far only produced the upper limits for the particular case of $^{87}$Rb [22]. In 2D systems the functional form of the sub-leading term is different from the 3D case, so it is difficult to compare with the 3D case. However, given that the precision improves continuously it should be possible to also probe the 2D case when tightly squeezing a 3D sample. As we have
shown here, the mass ratio can change the values of the contact parameters significantly. We thus expect that mixtures of different atoms is the most promising direction to make a measurement of a 2D contact parameter.

We have analyzed in detail two different systems of the heavy–heavy–light type that is relevant for current experiments with cold gas mixtures. In both cases the light particle is $^6$Li while the two heavy particles are either both $^{133}$Cs or both $^{39}$K. We find that, unlike the equal mass scenario, the two-body contact parameters are not universal constants when all the subsystems are interacting. Here, universal means that $C_2$ divided by the three-body binding energy is independent of which excited state is considered. However, if the two identical particles are not interacting, the heavy–heavy and the heavy–light two-body contact parameters become universal and are related to each other by a factor of two.

The methods presented here are in principle also applicable to 1D setups and it would be interesting to investigate the question of universality of the contact parameters for three-body states there as well. In some respects, 1D is easier to handle since zero-range interactions do not require regularization and one can in fact map the 3D scattering length to a 1D equivalent [37], which provides access to confinement-induced resonances that allow the study of the infinite 1D coupling strength limit. This was recently demonstrated for trapped few-fermion systems in 1D [40, 41]. In that case, the two-body contact can be determined fully analytically using the methods described in [38, 39]. It would be very interesting to consider the bosonic case where the three-body bound states are possible with or without an in-line trap. In the case of the quasi-1D setups where the transverse trapping energy is a relevant scale compared with the binding energies, one needs to also take into account the transverse (typically harmonic) degrees of freedom [23, 42]. Our formalism can be adapted to this case as well. Another interesting pursuit would be the long-range interactions using either heteronuclear molecules or atoms with large magnetic dipole moments [43], where the momentum distribution has in fact already been probed in the experiments [44]. Bound state formation has been predicted in both the single- [45], the bi- [46–48] and the multi-layer systems [49–51], as well as in one or several quasi-1D tubes [52–56]. The current formalism should be adaptable to dipolar particles and the contact parameters could subsequently be studied. In particular, in the limit of small binding energy one may in some cases use the effective short-range interaction terms to mimic the dipolar interactions [56], which makes the implementation through the Faddeev equations considerably simpler. This is of course also the limit in which the contact parameters are most interesting.

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